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A THEORY ON THE BENDING MODULI OF THIN MEMBRANES BY THE USE OF A SIMPLE MOLECULAR MODEL

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A simple molecular model of thin membranes was analyzed in order to evaluate the bending moduli of lipid membranes, in which the intermediate surface between the head and the tail of the molecule was introduced in order to reproduce the frustration of molecules. A new principle of the energy minimization with respect to the area and the position of the neutral surface has been shown to lead a correct conclusion on the current problem of the bending moduli of thin molecular membranes.

The elastic moduli of bending of monolayer and bilayer membranes are important for studying the various topologies of the membranes such as vesicle formation, spherical microemulsions, bicontinuous emulsions. Helfrich [1] described the elastic free energy surface density, f, of the bending of membranes as:

$$f = \frac{1}{2} k (c_x + c_y - c_0)^2 + k' c_x c_y \qquad (1)$$

where k and k' are the elastic moduli for cylindrical bending and saddle bending, respectively. The factors c_x and c_y are the principal curvatures of the membrane and c_0 is twice of the spontaneous curvature of the membrane [1]. The classical theory of elasticity can determine the two bending moduli, k and k', by the elastic moduli of materials [2]. For our thin membranes, the factors, k and k', and c_0 should be determined by the nature of composed molecules. Thus, their characteristics may have different properties compared with those estimated by the classical theory of elasticity when the membrane is in a liquid phase and when the molecules are frustrated (possess internal stresses even in equilibrium).

In order to analyze the liquid membrane with intramolecular frustration, we will employ the model free energy, the PDM model (Petrov-Derzhanski-Mitov model) [3], in which a molecule has a head and a tail with respective spontaneous areas and surface elasticities. The energy per molecule, ϕ, is written as [3]

$$\phi = \frac{\beta_H}{2} \left(A_H - A_H^0 \right)^2 + \frac{\beta_C}{2} \left(A_C - A_C^0 \right)^2 \qquad (2)$$

The equation states that the energy cost is a quadratic function of the deviations of the surface areas of head and tail (chain) from their spontaneous areas. Traditional idea to analyze Eq. (2) is that the area of the neutral surface of a curved surface is determined so as to coincide it with the surface area of a flat plane. The necessary minimization of the

free energy was absent when the membrane is bent. And the position of the neutral surface is determined so that the surface elasticity term and the bending term are decoupled. We revised the above traditional method and determined the area of the neutral surface and its position so as to minimize the free energy. As a result, the saddle bending modulus, k', turns out to be zero, which is physically reasonable because the free energy does not have any term that is resistant to shear. The other workers have been considering that both k and k' could be assumed rather arbitrarily as theoretical parameters. The conclusion we showed is that two bending moduli cannot be arbitrary constants but obeys the principle of mechanics.

The real molecular membrane differs from the classical elastic membrane. It is frustrated even in equilibrium. In other words, the molecules have internal stresses even if they assume a most favorable shape even in equilibrium. Such a situation is absent in the classical theory of elasticity. we added the intermediate surface in order to express the intramolecular frustration. The intermediate surfaces possess their own spontaneous area and elastic constant and interact one another also by the surface elasticity. The free energy is written as

$$\phi = \frac{\beta_H}{2}\left(A_H - A_H^0\right)^2 + \frac{\beta_C}{2}\left(A_C - A_C^0\right)^2 + \frac{\beta_G}{2}\left(A_G - A_G^0\right)^2 \qquad (3)$$

The last term of Eq. (3) is the term of the intermediate surface. Using this free energy, we obtained small but finite values of the saddle bending modulus both with positive and negative signs. Thus, the intramolecular frustration makes the membrane to possess the saddle bending modulus which fact cannot be understood from the classical theory of elasticity [4]. The position of the neutral surface, the spontaneous curvature and other physical quantities are also obtained according to our theory. For instance, the cylindrical modulus have its minimum value when the intermediate surface is at the center of the molecule which is reasonable because the internal torque against the external bending is minimum at the center of the molecule. The obtained spontaneous curvature is reasonably correlated to the geometry of the molecule. The analysis was done by numerical calculations. The authors acknowledge Professor S.A. Safran and Associate Professor T. Kawakatsu for their critical discussion on this problem.

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